Gradient Descent for Numerical MAX-CSPs

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1 Introduction

Many real world problems can be modeled as constraint satisfaction problems (CSPs), ranging from logic puzzles like sudoku to machine learning. Briefly, a constraint satisfaction problem is the task of finding a valid assignment of variables which satisfy a set of constraints. Many classic problems in theoretical computer science fit this model, such as the 3-SAT and circuit SAT problems. As such, large amounts of work have been devoted to studying CSPs and how to solve them, yielding many exact and approximation algorithms [11]. In this paper we examine a lesser studied variant of CSP, called numerical MAX-CSPs. In this variant each variable is a real number and all of the constraints are linear inequalities, the goal then is to satisfy as many linear inequalities as possible. We find that while it is less studied than other CSPs, numerical MAX-CSPs have direct applications to a variety real world problems, such as solving over-constrained LP's and tuning full text search engines.

The rest of this paper is structured as follows. We begin with background on the problem and the basis for our proposed solution. Next, we motivate our particular problem by tying it to an application of tuning a keyword search engine with labeled data. We then move on to describe a baseline solution by modeling the problem as mixed integer linear program and discuss the issues with this solution. Next, we present our algorithm and compare it to the baseline solution. Finally, we discuss the experimental results and give directions for future work.

2 Background

In this section we give a brief overview gradient descent which is the basis of our proposed algorithm. We then give an overview of constraint satisfaction problems, and the specific variant that we address in this paper.

2.1 Gradient Descent

Gradient descent is an optimization technique which has gained much attention in recent years due to its use in training neural networks for machine learning tasks such as computer vision and speech recognition. Despite the focus on machine learning, gradient descent is a general purpose optimization procedure capable of optimizing arbitrary differentiable functions. Many variations have been proposed in recent years, however each technique uses the same core idea. Given a function f to minimize and current point x, compute the gradient $\nabla(f(x))$ and update x by taking a step in a direction of $-\eta\nabla(f(x))$. Repeat this process until the minimum of the function is found.

If $f(x)$ is convex, then gradient descent is guaranteed to find the global minimum of the function (given that η is set to an appropriate constant). If $f(x)$ is not convex, then gradient descent will converge to a local minimum. Although in the non-convex case, gradient descent is not guaranteed, and frequently won't, find the global minimum, it is still useful for approximating the global minimum of functions which are cannot be handled by solvers. This makes it an invaluable tool for optimizing functions which don't admit exact optimization techniques such as those used for linear and quadratic programs.

2.2 CSPs and MAX-CSPs

Constraint satisfaction problems (CSPs) at a high level are problems that involve finding a valid assignment of variables which satisfy a set of constraints. Formally, a CSP is defined as a triple $\langle X, D, C\rangle$ [2], where

$$X = \{X_1, ..., X_n\} \text{ the set of variables}$$
$$D = \{D_1, ..., D_n\} \text{ the domains of each variable}$$
$$C = \{C_1, ..., C_m\} \text{ the set of constraints}$$

A classic example of a CSP, is the 3-SAT problem. In this problem, X_i corresponds to a boolean variable, which has domain $D_i = \{true, false\}$ and the constraints are all three variable disjunctive clauses. If we change the objective to satisfying as many constraints as possible we get the MAX-3-SAT problem which is a type of a MAX-CSP. More generally, a MAX-CSP is simply a CSP where the objective is to satisfy as many constraints as possible as opposed to being required to satisfy all constraints.

3 Related Work

In this paper we focus on a subset of MAX-CSPs called numerical MAX-CSPs. While MAX-CSPs have been studied extensively and there exist many approximation algorithms [11] for a variety of problems, most work has been focus on MAX-CSPs with finite domains (e.g. boolean assignment of variables). In contrast, we were only able to find one previous work that directly addresses numerical MAX-CSPs [12]. In this paper the authors propose an exact algorithm for solving numerical MAX-CSP instances. In particular, where $D_i = \mathbb{R}$ and each constraint $C_j = a_j^T x \leq b_j, a_j \in \mathbb{R}^n, b_j \in \mathbb{R}$. That is, given a set of linear inequalities, satisfy as many as possible. While the algorithm does produce optimal solutions, the algorithm is worst case exponential time, making it infeasible for large problems.

We note that this problem can be is readily formulated as a mixed integer linear program (MILP) with binary indicator variables. The general problem of mixed integer linear programming is NP-Hard (by reduction to 0-1 integer programming which is NP-Complete [7]). While there has been little work directly addressing numerical MAX-CSPs, there has been a large body of literature aiming to improve MILP solvers. In particular, there has been a lot of attention given to improving the branch and bound algorithms used by many MILP solvers. These improvements typically aim to provide better branching heuristics, such as strong branching [8]. More recent work has examined machine learning for better branching heuristics [3] [10], either to approximate strong branching using machine learning (to reduce the computation cost) or to learn completely new branching heuristics which will reduce the number of nodes explored to find an optimal solution.

4 Problem and Motivation

Numerical MAX-CSPs have a wide variety to applications from debugging infeasible linear programs to machine learning classification, however we are interested in one particular problem, which is tuning the weights for full text search engines. Full text search engines are the backbone of many data management and web applications and ergo are ubiquitous in everyday life. These search engines (such as Apache Lucene) are built for efficient retrieval of top-k documents based on a TF/IDF based scoring metric which is dot product between two sparse vectors $q^T d = score$[6] [4] [5]. While this default scoring gives decent results out of the box, it is frequently augmented by re-weighting the query q, with some weight vector w changing to scoring to be $(q \odot w)^T d = score$ (where $\odot$ is element-wise multiplication). This allows for boosting of certain terms or fields to improve the quality of search results while not changing the underlying search algorithm.

The problem is then to find a good non-negative weight vector w. In particular our problem setting is as follows. We are giving a set of query vectors $Q = \{q_1, ...q_n\}, q_i \in \mathbb{R}^n$. For each of these query vectors q_i we are given a set of k retrieved document vectors with labels $R_i = \{(d_{i,1}, l_{i,1}), ..., (d_{i,k}, l_{i,k})\}$, where, $d_i \in \mathbb{R}^n$ and $l \in \{relevant, irrelevant\}$. We wish to find a weight vector w that minimizes the number of irrelevant documents (search results) that are examined before the relevant document is found. This problem can be formulated as a mixed integer linear program (MILP) as follows,

$$\begin{aligned} \min_{w,z} \quad & 1^T z \\ s.t. \quad & Aw - \epsilon z \leq \gamma \\ & w \geq 0 \\ & z \in \{0, 1\} \end{aligned}$$

Where γ is a negative fixed constant, ϵ is a large positive constant for indicating constraint violation, and each row, a, of A comes corresponds to

$$a = (d_{i,y} - d_{i,x}) \odot q_i \quad i \in \{1, ...n\} \quad x, y \in \{1, ..., k\}, l_{i,x} = relevant, l_{i,y} = irrelevant$$

That is, the pairwise difference between the components of a matching and non-matching document, multiplied by the relevant query. We note that with this setup,

$$a^T w < 0 \implies (q \odot w)^T d_{i,x} > (q \odot w)^T d_{i,y}$$

In plain English, the relevant document will be scored higher than the non-relevant document for the query. Solving this MILP then corresponds to minimizing the number of irrelevant documents that need to be examined in order to find the relevant document for each query.

5 Baseline Solution

As mentioned above, we can formulate our problem as an MILP with binary constraints. This MILP can then be feed into any supported off the shelf solver to produce an optimal answer. This solution to our problem, which we will refer to as MILP when there is no ambiguity, is appealing because it will give an optimal solution, however it suffers from a few major drawbacks. First and foremost, depending on the input, the runtime time is worst case exponential in the number of constraints. Moreover, we found that even commercial solvers can struggle with large problem sizes, either taking large amounts of time to produce any feasible solution or simply not terminating in a reasonable amount of time. For our motivating use case, we would ideally feed in many labeled queries, each producing tens of constraints, hence exponential runtime in the number of constraints greatly reduces the usefulness of the solution.

6 Our Solution

To address the problems of the MILP algorithm, we propose a new algorithm based on gradient descent. The high level idea of the solution is simple, begin with a random feasible weight vector w and then perform gradient descent until the local minima is found. More specifically we minimize the following function,

$$f(w) = \langle \text{HardTanh}(Aw), \overrightarrow{1} \rangle$$

$$\text{Where } \gamma = -1 \text{ and } \text{HardTanh}(x) = \begin{cases} -1 \text{ if } x \leq -1 \\ 1 \text{ if } x \geq 1 \\ x \text{ otherwise} \end{cases}$$

By applying HardTanh, we change the 0-1 loss from the MILP formulation into a continuous differentiable function, which allows for gradient descent to be applied to the function.

Algorithm 1 OptimizeGD(f, T)

Input : The function f to optimize, the time limit T
Output : A local minimum w^*

$w^* \leftarrow \overrightarrow{0}$
while current time $< T$ **do**
  $w \leftarrow w \sim \mathbb{U}^n_{[.1,1.1]}$ // Initialize w to a uniform random vector
  for $i = 1, ...20$ **do**
    for $j = 1, ...25$ **do**
      $w \leftarrow w - \text{ADAM}(\nabla f(w))$
      $w \leftarrow (\max\{0, w_1\}, ..., \max\{0, w_n\})$ // Make all elements of w non-negative
    end for
    if $f(w) < f(w^*)$ **then**
      $w^* \leftarrow w$ // Update best solution every 25 gradient updates
    end if
  end for
end while
return w^*

For our implementation we use PyTorch [13] for its high performance and flexibility. For gradient updates we use the ADAM gradient descent algorithm with default parameters [9] because we empirically found it to perform well relative to other available gradient descent algorithms, while giving minimal overhead. [1]

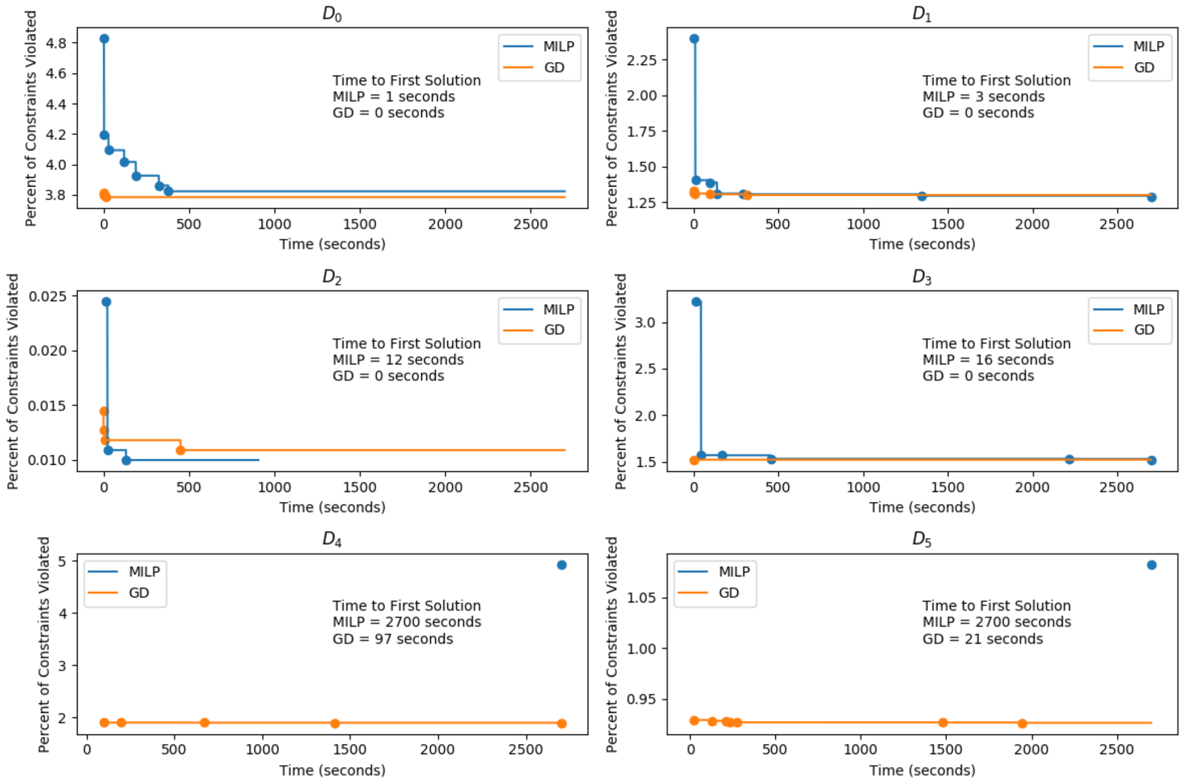
7 Experiments

We ran our experiments on a server with an AMD Ryzen Threadripper 2950X (16c/32t) processor with 64GB of RAM running pop_os 18.04. Our numerical MAX-CSP instances are generated from real world datasets, with the number of constraints ranging from 7.7K to 6.0M. For MILP we leverage Gurobi, a commercial solver with an academic license. We choose Gurobi because it is consistently one of the top performing solvers [1] with an academic or free license. Both solutions where given a timeout of 2700 seconds, corresponding to 24 hours of CPU time with 32 threads.

Table 1: Dataset statistics

Dataset	# of Constraints	# of Columns	% Non-Zero
D_0	7.7K	14	66.24
D_1	19.3K	18	61.46
D_2	111.9K	18	72.83
D_3	196.2K	30	51.62
D_4	3.7M	124	25.09
D_5	6.0M	22	68.58

Figure 1: Comparison of MILP vs. Gradient Descent (GD)



[1]Code can be found at https://github.com/derekpaulsen/cs787

8 Discussion

In this section we discuss the two major takeaways from the experimental results, the quality of solutions produced and the scalability of the algorithms.

8.1 Quality of Solutions

Much to our surprise, the quality of solutions produced by gradient descent (GD) were very similar, and in some cases even better, than MILP. We attribute this to the fact that only a single dataset was solved to optimality in the allotted time (D_2) with MILP. In fact, despite having an order of magnitude fewer constraints then D_2, MILP was unable to produce an optimal solution to D_0 in 12 hours. This underlines up a key trade off between the solutions, namely, quality of solutions vs. runtime predictability. While MILP will produce an optimal solution given enough time and memory, it is very hard to predict how long it will take to produce an optimal solution. In contrast, there are no guarantees that can be made about GD in terms of the quality of solutions but its runtime is very predictable, scaling linearly with the number of constraints times the number of columns.

8.2 Scalability

This brings us to our second major point which is the scalability of the solutions. Examination of the results for D_4 and D_5, we can clearly see that GD has superior scaling properties when compared to MILP in terms of runtime. On both datasets, MILP timed out on both datasets before even beginning to refine the solution produced, where GD produced a feasible solution in less than two minutes. We attribute this disparity to the vastly different computational complexity of the two algorithms. GD has linear complexity in the number of constraints in contrast to MILP which has best case polynomial complexity in the number of constraints. For small problems this not an issue, but as the problem size increases MILP quickly becomes impractical even for approximating the optimal solution. Additionally, in order to make the comparison fair, we ran both solutions on the CPU, however there is nothing to prevent GD from being run on a GPU. Leveraging GPU compute has the potential to greatly decrease the iteration time on larger datasets, which would decrease the time to produce a feasible solution and likely improve the quality of results.

9 Future Work

We identify multiple directions for future work, which fall into two categories, optimization techniques, and problem applications.

9.1 Optimization Techniques

In this paper we have only taken a small look at the possible optimization techniques that could be applied. The most obvious variation that could experimented with is stochastic gradient descent. This variation has the potential for two major benefits. First, it can decrease both runtime and memory requirements of the solution by no longer requiring the entire dataset be processed on each gradient update. Second, the stochastic version may be able to find better solutions as it is much more likely that it could escape worse local minima, instead of relying mostly on having a good starting point.

9.2 Problem Applications

We restricted our problem setting to numerical MAX-CSPs with linear constraints, however in principle there is no reason why this technique could not be applied to more complex constraints. In particular, non-convex constraints (e.g. polynomials of degree greater than 2) would potentially be solved by applying similar techniques, which current solvers are not able to handle in any capacity. We believe that it is likely that modifying the optimization procedure, such as using stochastic gradient descent, will likely be required to provide good approximations of such functions.

10 Conclusion

In this work we have taken brief look at numerical MAX-CSPs, motivated by a real world use case for tuning full text search engines with labeled data. We then proposed an algorithm based on gradient descent and ran preliminary experiments that show it has some key advantages over the baseline MILP based solution, especially for large problem instances, where commercial solvers are too slow to be practical. We believe that our solution shows promise for finding approximate solutions to problem instances which were not previously tractable with traditional optimization techniques. Future work should continue to explore the possible variations of the gradient descent algorithm and explore applying the technique to related problems.

References

[1] Decision tree for optimization software. URL http://plato.asu.edu/bench.html.

[2] Constraint satisfaction problem, Feb 2022. URL https://en.wikipedia.org/wiki/Constraint_satisfaction_problem.

[3] Y. Bengio, A. Lodi, and A. Prouvost. Machine learning for combinatorial optimization: A methodological tour dhorizon. *European Journal of Operational Research*, 290(2):405421, 2021. doi: 10.1016/j.ejor.2020.07.063.

[4] A. Z. Broder, D. Carmel, M. Herscovici, A. Soffer, and J. Zien. Efficient query evaluation using a two-level retrieval process. *Proceedings of the twelfth international conference on Information and knowledge management - CIKM '03*, 2003. doi: 10.1145/956863.956944.

[5] S. Ding and T. Suel. Faster top-k document retrieval using block-max indexes. *Proceedings of the 34th international ACM SIGIR conference on Research and development in Information - SIGIR '11*, 2011. doi: 10.1145/2009916.2010048.

[6] A. Grand, R. Muir, J. Ferenczi, and J. Lin. From maxscore to block-max wand: The story of how lucene significantly improved query evaluation performance. *Lecture Notes in Computer Science*, page 2027, 2020. doi: 10.1007/978-3-030-45442-5_3.

[7] R. M. Karp. Reducibility among combinatorial problems. *Complexity of Computer Computations*, page 85103, 1972. doi: 10.1007/978-1-4684-2001-2_9.

[8] E. B. Khalil, P. L. Bodic, L. Song, G. Nemhauser, and B. Dilkina. Learning to branch in mixed integer programming. In *Proceedings of the Thirtieth AAAI Conference on Artificial Intelligence*, AAAI'16, page 724731. AAAI Press, 2016.

[9] D. P. Kingma and J. Ba. Adam: A method for stochastic optimization, 2014. URL https://arxiv.org/abs/1412.6980.

[10] G. D. Liberto, S. Kadioglu, K. Leo, and Y. Malitsky. Dash: Dynamic approach for switching heuristics. *European Journal of Operational Research*, 248(3):943953, 2016. doi: 10.1016/j.ejor.2015.08.018.

[11] K. Makarychev and Y. Makarychev. Approximation Algorithms for CSPs. In A. Krokhin and S. Zivny, editors, *The Constraint Satisfaction Problem: Complexity and Approximability*, volume 7 of *Dagstuhl Follow-Ups*, pages 287–325. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, Dagstuhl, Germany, 2017. ISBN 978-3-95977-003-3. doi: 10.4230/DFU.Vol7.15301.287. URL http://drops.dagstuhl.de/opus/volltexte/2017/6968.

[12] J.-M. Normand, A. Goldsztejn, M. Christie, and F. Benhamou. A branch and bound algorithm for numerical max-csp. *Constraints*, 15(2):213237, 2009. doi: 10.1007/s10601-009-9084-1.

[13] A. Paszke, S. Gross, F. Massa, A. Lerer, J. Bradbury, G. Chanan, T. Killeen, Z. Lin, N. Gimelshein, L. Antiga, A. Desmaison, A. Kopf, E. Yang, Z. DeVito, M. Raison, A. Tejani, S. Chilamkurthy, B. Steiner, L. Fang, J. Bai, and S. Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 8024–8035. Curran Associates, Inc., 2019. URL http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf.